

Hybrid Scheme for Glassy Ion Dynamics

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Abstract—Ion dynamics has largely focusing on statistical analysis of collected data from experimental or simulation results. But unfortunately, the details of the structure-transport relationships in the data have been flout in favour of ensemble average. In specifically, we deliberate a simulated 3D time-varying model of ion dynamic in glass structure and scrutinize the spatio-temporal relationship among ion dynamics. Our main aims to conceive effective representations to sustain physicist in pinpoint probability of collaborative behaviours with their spatio-temporal correlation among convoluted and seemingly messy molecule movements in ion dynamics. But it is not possible at moment. Here, we highlight the broad issues of representing ion dynamics in glassy with relation to timeline events. We put forward a hybrid scheme that used 3D glyphs for representing orientation of ion dynamic, colour scale with codeword for portray the timeline events and opacity for collaborative events. With an anthology of the schemes, we illustrated that this scheme would be able to propose an efficient tool for visually mining for whichever 3-dimensional time-varying datasets.

Keywords: hybrid system and their applications, coding theory, colour scale, visualisation, time-varying data, spatio-temporal visualisation, molecular dynamics, scientific data, visual representation

I. INTRODUCTION

A spatio-temporal data set is a collection of data where data values vary in both space and time. Abstractly, such a data set can be considered as a (continuous and discrete) specification of a function, $F: \mathbb{E}^d \times \mathbb{T} \rightarrow \mathbb{R}^n$, where \mathbb{E}^d denotes d-dimensional Euclidean space, $\mathbb{T} = \mathbb{R}^* \cap \{\infty\}$ the domain of time, and \mathbb{R}^n an n-dimensional scalar field. Examples of such data sets include time-varying simulation results, films and videos, time-varying medical scans, geometrical models with motion or deformation, meteorological measurements and many more.

Many researchers have recently developed a molecular dynamic (MD) simulation package [15] [17] [1]. Instead of development of simulation package there are also proposed techniques for analysis like Mehta et al. [16] proposed a technique for detection and visualise the anomalous structure of MD simulation data. And there many works have been done previously on analysing MD datasets [22] [8] [14].

During analysis, some of the data sets could be very big such as Beazleay and Lomdahl [3] were presented the method that can be used for very large scale molecular dynamic simulation. Meanwhile, Zhu et al. [22] were presented a grid technology and parallel rendering approach for visualising a massive molecular datasets.

There are evidences that MD simulation is used for specific purpose. Best and Hege [4] visualise a trajectory of the molecule *adenylyl(3'-5')cytidyl(3'-5')cytidin* which is called $r(ACC)$. They used a statistic algorithm to help biochemist to learn about the molecule bases of biochemical processes. Some of the researcher focus on protein dynamics [18], gases [2], polymer [20], meta-stable liquids [19] and glassy [7].

Bulatov and Grimes [5] used a video visualisation technique called MPEG-based method to generating a video clips that depict the animated movement of atoms. However, viewing animation or movies in general is a time-consuming and resources-consuming process.

To extract meaningful datasets, Imada et al. [11] introduced automated histogram filtering (AHF) for time complexity analysis on protein structure elucidation. This technique most closely to the statistical clustering technique [6] [12] [13] that had been used for analysis of molecular dynamic trajectories. While, Best and Hege [4] developed a method called planar map. Basically, they constructed a 2D map of the trajectory that can reveal conformational ensembles and applied a cluster analysis procedure that allows for the automatic identification of the cluster. They used a line to connect all the points in 2D-dimensional map and they combine some of the point to form ellipsoid. This method will modify some of the interesting point in our works which is the main objective to visualise a timeline events of ion trajectories.

Instead of clustering or grouping the trajectories, Huitema and van Liere [10] filter out uninteresting atom motion from the larger concerted motions. Same with Wiley et al. [21], they used a similar approach with fourier and hilbert method for filtering a frequency of sample trajectory. Horiuchi and Go [9] also used a similar approach on molecular dynamic trajectories to extract the lowest frequency mode from the simulation data. The method shown by Huitema, Horiuchi and Wiley will remove some of the interesting trajectory which is critical to our main purpose to visualise a timeline of trajectories.

In this paper, we introduced a method to visualise a timeline of ion dynamics in glassy. To represent the orientation of ions we used a vector glyph and cylinder to connect each of the points. This method could not give the timeline of trajectories but it can represent the movement of ions in 3D space. To achieve our aims, we introduced a method called colour scale and colour number coding scheme to represent a series of timelines on ion trajectories. At the end, we hope through this method a viewer especially physicists would be able to

interpret and analysis the ion dynamic in glasses.

The ability to convey temporal as well as spatial information is critical in our particular application, where the physicists need a visual representations that can effectively highlight the correlation between different ions in their motions among seemingly chaotic trajectories especially in collaborative events. This particular challenging requirement provided this work with the principal motivation.

In the rest of this paper, we will describe the application concern and scientific background in Section 2. In this section, we will first examine the methods that can convey orientation information to viewers. We will devote most of our focus to the visualisation of temporal information in order to confirm and identify the time series activities in the data sets. In Section 2 as well, we will present some examples results of visual data mining process on testing trajectories, which will be followed by our concluding remarks in Section 3.

II. VISUALISING ION DYNAMICS

In this section, we will first examine the more challenging task for visualising temporal information in order to identify the series of events and collaborative events. We will discuss the use of glyph, colour and opacity in our visual representations and present the methods for constructing and rendering composite visualisation that convey a rich a collection of indistinguishable visual features for assisting in a visual data mining process.

A. Orientation

Given an ion trajectory as a series of $n + 1$ points, p_0, p_1, \dots, p_n , we have n consecutive vector segments, v_1, v_2, \dots, v_n , where $v_i = (p_i - p_{i-1})$. One can visualise such a trajectory using streamlines or vector glyphs.

In Figure 1, even though each conical glyph, which represents a vector segment, depict the instantaneous velocity at a given time interval with its length and the direction of the motion with its pointer but it does not much help to visualise a time series events and collaborative issues in ion dynamic without the combination of colour scale. In the next section, we will shows the colour scale can give more understandable about time series events in ion dynamics.



Fig. 1. A trajectory of sodium #169

B. Temporal Information

When using visualisation to summarise a series of events along a timeline, perhaps the most difficult task is to associate a particular event with a precise moment on the timeline. This is useful not only determine the time of an event but also for the identification corresponding parties involved in collaborative, but collaborative events is not included at moment.

1) *Global Colour Scale*: In order to shows the global timeline of events on streamline, we introduced *Global Key Colours Scale*. In this scheme, we use a small set of colour, c_1, c_2, \dots, c_k ($k > 1$), then we assigned a colours to specific vector in the vector series :

$$\begin{array}{cccccc} v_1 & v_u & \dots & v_v & \dots & v_n \\ c_1 & c_2 & \dots & c_i & \dots & c_k \end{array}$$

where indices such as u and v are pre-determined. For each vector that has not assigned a colour we obtain a colour by interpolating the two nearest neighbours with the specified key colours in each direction. This scheme allow a viewer to determine a time frame at a global scale with the help of key colours. In Figure 2, we chosen seven key colour which from rainbow colour to visualise global scale of time series. At local level the interpolation can make different vector segment indistinguishable. Moreover, it is possible to have the same or similar interpolated colours between different sets of consecutive key colours.

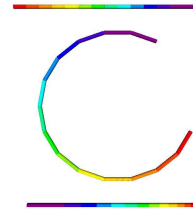


Fig. 2. Seven Key Colours on testing trajectories.

2) *Local Colour Scale*: In order to correlate each vector segment with the timeline more accurately and hence to improve the differentiation of different vector segments, we introduce a Colour Number Coding Scheme in our visualisation.

Given a small set of key colours, c_1, c_2, \dots, c_k ($k > 1$) and distinctive interval-colour (e.g., while, black or grey depending on the background colour), we code a group of consecutive m vectors as a k -nary number, terminated by a vector in the interval-colour. Given n as the total number of vectors and we always assign the interval-colour to the first vector, we need to find the smallest integer m that satisfies Equation 1;

$$((m + 1)k^m) \geq n \quad (1)$$

For instance, when $n = 1000$, using two key colours, say red and green, we need in $m = 7$ colour digits. We have $m = 5$ for $k = 3$, $m = 4$ for $k = 4$, and $m = 2$ when k reaches 19. The selection of m and k needs to address the

balance between a smaller number of colours or a smaller number of colour digits in each group of vectors. The former ensures more distinguishable colours in visualisation, and the latter reduces the deductive effort for determine the temporal position of each vector. Figure 3 shows a binary colour coding scheme for ion tracks with 16 vectors.

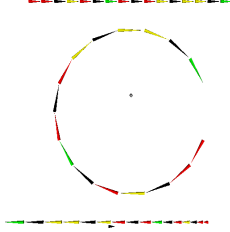


Fig. 3. Colour Number Coding Scheme on testing trajectories.

III. COLLABORATIVE ION DYNAMICS

When collaborative events takes place between ions in the simulation results then the possible method that we could used is opacity scheme. But the details of this scheme, implementation and result will become the future works of this study. Even in this paper we are not focusing on collaborative events but we extended a brief regarding transfer function that could be possible in our application.

By combining all the above methods, we provide an effective visual representation for visualising collaborative ion dynamic. Figure 4 shows the example of collaborative events in ion dynamics.

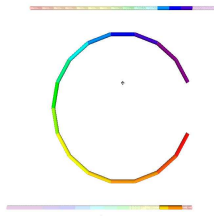


Fig. 4. Combination of visualisation on testing trajectories.

The main objectives of this task is to discover if collaboration is exhibited between ions in the simulation results. As described previously, there is not well-defined description about collaboration events, although experiments suggested the existence of collaboration phenomena. We, including the physicists involved, did not know in what form a collaborative event may display, in what way ions may cooperate with each others or what event may cause ions entering in or disengaging from collaboration. Therefore we have introduced a variable, ψ , representing the probability of collaboration. Given a set of m hypothesized criteria of collaboration, we have :

$$\psi = \omega_1\psi_1 + \omega_2\psi_2 + \dots + \omega_m\psi_m \quad (2)$$

where ω_i is the weight of criterion i , and $\psi_1 + \psi_2 + \dots + \psi_m = 1$. In this work, we have considered three such criteria, namely

(1) the ability for two or more ions to maintain similar orientation, (2) the ability for two or more ions to maintain similar velocity, and (3) the ability for two or more ions maintain constant gap between them.

Given two corresponding vector segments, $v_{a,i}$ and $v_{b,i}$, belonging to two different ion trajectories, we have:

$$\psi_1 = \left(\frac{1}{2} \left(\frac{v_{a,i} \bullet v_{b,i}}{|v_{a,i}| |v_{b,i}|} \right) \right)^{D_1} \quad (3)$$

where $D_1 \geq 0$ is de-highlighting factor. The larger the D_1 is, the less probable a vector is considered being involved in collaboration. With ψ_1 , $v_{a,i}$ and $v_{b,i}$ are considered to be in collaboration, if they follow a similar direction.

Once we have computed $\psi \in [0, 1]$, we can highlight or dehighlight the corresponding vector segments. Two different methods of highlighting the probability of collaboration are shown in Figure 5. We chosen a small sample because it is easy for clarification purpose. In (a), (c) and (e), we apply an opacity of tube around the glyphs with a high ψ value, which in effect defines the opacity of the tube. In (b), (d) and (f), we use the value of ψ to modify the size and opacity of the corresponding tube and vector segment . Where there is a high probability of collaboration, the tube and vector glyphs are fully opaque, where there is a low probability, they are almost totally transparent. The second method seems to convey information with more certainty to human observer.

In Figure 5, (a) and (b) show the probability computed using ψ_1 only between each of the straight trajectories with the central circular trajectory. Similarly, (c) and (d) are computed using ψ_2 only, and (e) and (f) using ψ_3 . Our testing trajectories help illustrate the effectiveness of the three criteria. For example, in (a) and (b), two particles are marked as cooperating if they are moving in the same direction at the same time. In this way, the top track is cooperating near the end and the bottom track near beginning. In images (c) and (d), the top particles is barely cooperating with that on the central loop at all, as they travelling at a constant but different speed. The bottom track is to degree at the end of its run, but not at all at the beginning. In (e) and (f), two particles are considered as cooperating if they maintain a fixed distance apart over time. Without highlighting and de-highlighting based on ψ_3 , it would be difficult to observer this phenomena directly.

By combining some above-mentioned methods together, we provide an effective visual representation for visualising spatio-temporal collaboration. With the help of global colour scale, viewers can determine the global time frame of the events, for example, $t = 0$ can be easily found between two consecutive colour. For more details, local colour scale will help to determine which corresponding ions in collaboration. These will give such an idea to our future works to enhance the capability in helping the physicists to determine the corresponding parties involved in collaboration issues.

IV. CONCLUSION

We developed an effective visual representation, which have combined from several schemes including glyph for

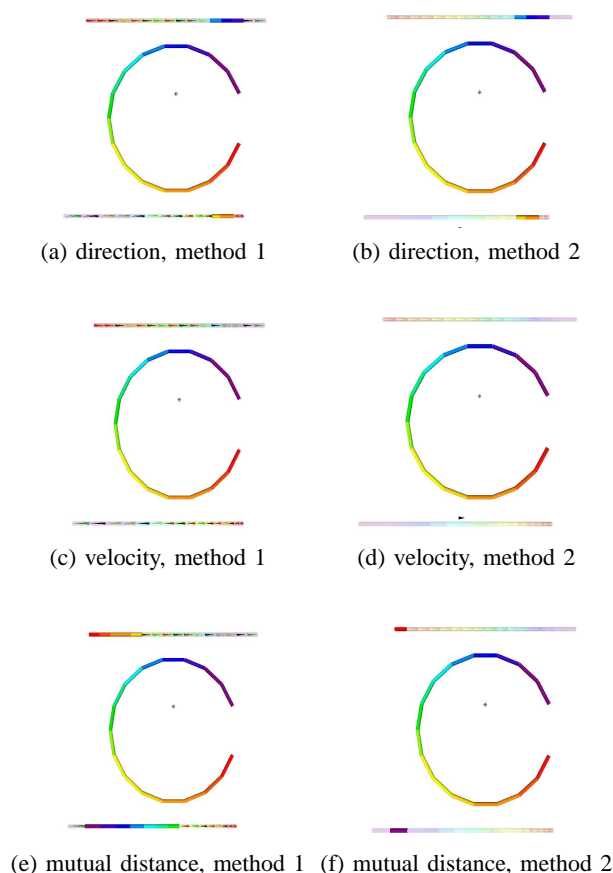


Fig. 5. Collaborative method

orientation, colour scale for time series events and opacity scheme for collaborative method. Again, all these schemes can be beneficial also in another field of study like biophysics, biological, bioinformatics or any collaboration events especially in time-varying events. In the future works, we plan to extend the works in conveying temporal information in a high degree of certainty before we go further on visualising collaborative events in ion dynamics.

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